

# Dynamic properties of spin- $\frac{1}{2}$ $XY$ chains

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## Abstract

We have considered a numerical scheme for the calculation of the equilibrium properties of spin- $\frac{1}{2}$   $XY$  chains. Within its frames it is necessary to solve in the last resort only the  $2N \times 2N$  eigenvalue and eigenvector problem but not the  $2^N \times 2^N$  one as for an arbitrary system consisting of  $N$  spins  $\frac{1}{2}$ . To illustrate the approach we have presented some new results. Namely, the  $xx$  dynamic structure factor for the Ising model in transverse field, the density of states for the isotropic chain with random intersite couplings and transverse fields that linearly depend on the surrounding couplings, and the  $zz$  dynamic structure factor for the Ising model in random transverse field. The results obtained are hoped to be useful for an interpretation of observable data for one-dimensional spin- $\frac{1}{2}$   $XY$  substances.

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Statistical mechanics of the one-dimensional spin- $\frac{1}{2}$   $XY$  models has a history going back more than three decades to the pioneering paper by Lieb, Schultz and Mattis [1] in which it was noted that such systems are as a matter of fact the non-interacting spinless fermions and therefore, a lot of statistical mechanics calculations can be performed exactly. Although many papers concerning thermodynamics, spin correlations and their dynamics have appeared since that time, several problems still call for efforts. One of them regards the study of spin dynamics: in contrast to the time-dependent correlation function between  $z$ -components of two spins [2], the  $xx$  time-dependent correlation function has been derived exactly only in some limiting cases ( $T = 0$ , the critical value of transverse field,  $T = \infty$ ) [3-9]. Some recent attempts to calculate this correlation function are presented in Refs. [10-14]. New difficulties arose when the one-dimensional spin- $\frac{1}{2}$   $XY$  models were started to be discussed in random versions. The analytical results obtained here are not so impressive as for the perfect case and they are restricted to special types of disorder [15-20] or renormalization-group analysis [21]. A discovery of the quasi-one-dimensional spin- $\frac{1}{2}$  systems ( $\text{Cs}(\text{H}_{1-x}\text{D}_x)_2\text{PO}_4$ ,  $\text{PbH}_{1-x}\text{D}_x\text{PO}_4$ ,  $\text{PrCl}_3$ ,  $\text{CsCuCl}_3$ ,  $\text{CsCu}_{1-x}\text{Mn}_x\text{Cl}_3$ ,  $J$ -aggregates etc.) gave arise to additional interest in such calculations since a lot of data obtained in the dynamic experiments for such materials are available. Some approximate studies of dynamic properties were inspired by corresponding measurements [22-27], however, such estimations contain uncontrolled mistakes. Additional interest in such calculations was caused by the very recent studies of quantum phase transitions in disordered systems [21,28-30].

Since there are notorious difficulties in the analytical study of some properties of the spin- $\frac{1}{2}$   $XY$  chains it is naturally to try to obtain the desired results numerically. Few earlier attempts [31,32] faced the  $2^N \times 2^N$  eigenvalue and eigenvector problem that restricted the computations to  $N \sim 10$ . However, a peculiarity of spin- $\frac{1}{2}$   $XY$  chains provides an evident possibility to compute all equilibrium quantities facing in the last resort only the  $2N \times 2N$  eigenvalue and eigenvector problem [33-35]. This fact allows to consider rather long chains ( $N \sim 100 - 10000$ ) and therefore to study reliably the dynamics of spin correlations or the influence of disorder on observable properties. In this paper we shall briefly explain such a numerical approach for calculation of the equilibrium properties of the spin- $\frac{1}{2}$   $XY$  chains. Besides we shall demonstrate how does the approach work computing for this purpose the  $xx$  dynamic structure factor of the transverse Ising model and some thermodynamic and dynamic properties of several random  $XY$  models.

We shall consider  $N$  spins one-half arranged in a row with the following Hamiltonian

$$H = \sum_{j=1}^N \Omega_j s_j^z + \sum_{j=1}^{N-1} \sum_{\alpha, \beta=x,y} J_j^{\alpha\beta} s_j^\alpha s_{j+1}^\beta \quad (1)$$

where  $\Omega_j$  is the transverse field at site  $j$  and  $J_j^{\alpha\beta}$  is the interaction between  $\alpha$  and  $\beta$  spin components at the sites  $j$  and  $j + 1$ . Introducing instead of the spin raising and lowering

operators via the Jordan-Wigner transformation the Fermi operators  $c_j^\dagger, c_j$  one finds that the Hamiltonian (1) is a bilinear fermion form that can be put into diagonal form by linear transformation  $\eta_k^+ = \sum_{j=1}^N (h_{kj}^* c_j + g_{kj}^* c_j^\dagger)$ . Similarly to [1] it can be shown that if

$$(\mathbf{g}_k, \mathbf{h}_k) \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B}^* & -\mathbf{A}^* \end{pmatrix} = \Lambda_k(\mathbf{g}_k, \mathbf{h}_k) \quad (2)$$

with  $\mathbf{g}_k \equiv (g_{k1}, \dots, g_{kN})$ ,  $\mathbf{h}_k \equiv (h_{k1}, \dots, h_{kN})$ ,  $A_{ij} \equiv \Omega_i \delta_{ij} + J_i^{+-} \delta_{j,i+1} + J_{i-1}^{-+} \delta_{j,i-1}$ ,  $B_{ij} \equiv J_i^{++} \delta_{j,i+1} - J_{i-1}^{++} \delta_{j,i-1}$  and  $J_j^{+-} \equiv \frac{1}{4}[J_j^{xx} + J_j^{yy} + i(J_j^{xy} - J_j^{yx})] = J_j^{-+*}$ ,  $J_j^{++} \equiv \frac{1}{4}[J_j^{xx} - J_j^{yy} - i(J_j^{xy} + J_j^{yx})]$  the Hamiltonian transforms into  $H = \sum_{k=1}^N \Lambda_k (\eta_k^+ \eta_k - \frac{1}{2})$ . Evidently, the knowledge of  $\Lambda_k$ s or their distribution  $\rho(E) \equiv \frac{1}{N} \sum_{k=1}^N \delta(E - \Lambda_k)$  yields thermodynamics of the spin system (1). For the calculation of spin correlation functions it is convenient to introduce the auxiliary operators  $\varphi_j^+ \equiv c_j^+ + c_j = \sum_{p=1}^N (\Phi_{pj} \eta_p^+ + \Phi_{pj}^* \eta_p)$  and  $\varphi_j^- \equiv c_j^+ - c_j = \sum_{p=1}^N (\Psi_{pj} \eta_p^+ - \Psi_{pj}^* \eta_p)$ , where  $\Phi_{pj} \equiv g_{pj} + h_{pj}$ ,  $\Psi_{pj} \equiv g_{pj} - h_{pj}$ . Since  $s_j^x = \frac{1}{2} \varphi_1^+ \varphi_1^- \dots \varphi_{j-1}^+ \varphi_{j-1}^- \varphi_j^+$ ,  $s_j^y = \frac{1}{2i} \varphi_1^+ \varphi_1^- \dots \varphi_{j-1}^+ \varphi_{j-1}^- \varphi_j^-$  and  $s_j^z = -\frac{1}{2} \varphi_j^+ \varphi_j^-$ , the calculation of thermodynamic average of a product of spin operators reduces to exploiting the Wick-Bloch-de Dominicis theorem with the result that is in fact the Pfaffian of corresponding antisymmetric matrix constructed from the elementary contractions

$$\begin{aligned} \langle \varphi_j^+(t) \varphi_m^+ \rangle &= \sum_{p=1}^N \left[ \frac{\Phi_{pj} \Phi_{pm}^*}{\mathcal{F}(\Lambda_p)} + \frac{\Phi_{pj}^* \Phi_{pm}}{\mathcal{F}(-\Lambda_p)} \right], \\ \langle \varphi_j^+(t) \varphi_m^- \rangle &= \sum_{p=1}^N \left[ -\frac{\Phi_{pj} \Psi_{pm}^*}{\mathcal{F}(\Lambda_p)} + \frac{\Phi_{pj}^* \Psi_{pm}}{\mathcal{F}(-\Lambda_p)} \right], \\ \langle \varphi_j^-(t) \varphi_m^+ \rangle &= \sum_{p=1}^N \left[ \frac{\Psi_{pj} \Phi_{pm}^*}{\mathcal{F}(\Lambda_p)} - \frac{\Psi_{pj}^* \Phi_{pm}}{\mathcal{F}(-\Lambda_p)} \right], \\ \langle \varphi_j^-(t) \varphi_m^- \rangle &= -\sum_{p=1}^N \left[ \frac{\Psi_{pj} \Psi_{pm}^*}{\mathcal{F}(\Lambda_p)} + \frac{\Psi_{pj}^* \Psi_{pm}}{\mathcal{F}(-\Lambda_p)} \right] \end{aligned}$$

with  $\mathcal{F}(x) \equiv (1 + e^{\beta x}) e^{-i x t}$ . Thus, the solution of the  $2N \times 2N$  eigenvalue and eigenvector problem (2) completely determines thermodynamics, spin correlations and their dynamics for the model (1).

In what follows we have collected several new results obtained within the frames of the described approach. We shall start from the  $xx$  dynamic structure factor  $S_{xx}(\kappa, \omega) \equiv \sum_{n=1}^N e^{i \kappa n} \int_{-\infty}^{\infty} dt e^{-\varepsilon |t|} e^{i \omega t} \langle s_j^x(t) s_{j+n}^x \rangle$  for the uniform transverse Ising chain ( $\Omega_j = \Omega = 0.2$ ,  $J_j^{xx} = J = -1$ ,  $J_j^{xy} = J_j^{yx} = J_j^{yy} = 0$ ). At first we solved the eigenvalue and eigenvector problem (2) for  $N = 280$  obtaining in result  $\Lambda_k, \Phi_{kj}, \Psi_{kj}$ . Then for several values of temperature we calculated the required elementary contractions and computed the relevant Pfaffian

$$\langle s_{32}^x(t) s_{32+n}^x \rangle = \frac{1}{4} \langle \varphi_1^+(t) \varphi_1^-(t) \dots \varphi_{31}^+(t) \varphi_{31}^-(t) \varphi_{32}^+(t) \varphi_1^+ \varphi_1^- \dots \varphi_{32+n-1}^+(t) \varphi_{32+n-1}^-(t) \varphi_{32+n}^+(t) \rangle$$

$$= \text{Pf} \begin{pmatrix} 0 & \langle \varphi_1^+ \varphi_1^- \rangle & \langle \varphi_1^+ \varphi_2^+ \rangle & \cdots & \langle \varphi_1^+(t) \varphi_{32+n}^+ \rangle \\ -\langle \varphi_1^+ \varphi_1^- \rangle & 0 & \langle \varphi_1^- \varphi_2^+ \rangle & \cdots & \langle \varphi_1^-(t) \varphi_{32+n}^+ \rangle \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ -\langle \varphi_1^+(t) \varphi_{32+n}^+ \rangle & -\langle \varphi_1^-(t) \varphi_{32+n}^+ \rangle & -\langle \varphi_2^+(t) \varphi_{32+n}^+ \rangle & \cdots & 0 \end{pmatrix}.$$

At last we performed the integration over the time up to  $t = 1600$  with  $\varepsilon = 0.001$  and took into account in the sum over  $n$  up to 100 neighbours. The obtained dependences  $S_{xx}(\kappa, \omega)$  vs.  $\omega$  for different  $\kappa$  at low temperature and  $S_{xx}(0, \omega)$  vs.  $\omega$  for few temperatures are depicted in Fig. 1. As it can be seen from Fig. 1  $S_{xx}(\kappa, \omega)$  exhibits two peaks. At  $\beta = 5$  and  $\kappa = 0$  one finds a high peak at  $\omega_1 = 0.00$  and a low and broad one at  $\omega_2 = 0.76$ . As  $\kappa$  increases the height of the first peak decreases and it shifts towards high frequencies ( $\omega_1 \approx 0.11$  at  $\kappa = \frac{\pi}{4}$ ,  $\omega_1 \approx 0.25$  at  $\kappa = \frac{\pi}{2}$ ,  $\omega_1 \approx 0.34$  at  $\kappa = \frac{3\pi}{4}$ ,  $\omega_1 \approx 0.38$  at  $\kappa = \pi$ ), whereas the width of the second peak decreases, its height increases and it moves towards high frequencies ( $\omega_2 \approx 0.80$  at  $\kappa = \frac{\pi}{4}$ ,  $\omega_2 \approx 0.88$  at  $\kappa = \frac{\pi}{2}$ ,  $\omega_2 \approx 0.96$  at  $\kappa = \frac{3\pi}{4}$ ,  $\omega_2 \approx 1.01$  at  $\kappa = \pi$ ). As the temperature increases  $S_{xx}(0, \omega)$  qualitatively remains the same: the heights of both peaks decrease and the high-frequency peak shifts slightly towards high frequencies ( $\omega_2 \approx 0.76$  at  $\beta = 5$ ,  $\omega_2 \approx 0.77$  at  $\beta = 4$ ,  $\omega_2 \approx 0.81$  at  $\beta = 3$ ,  $\omega_2 \approx 0.86$  at  $\beta = 2$ ,  $\omega_2 \approx 0.91$  at  $\beta = 1$ ,  $\omega_2 \approx 0.95$  at  $\beta = 0.1$ ,  $\omega_2 \approx 0.96$  at  $\beta = 0.001$ ). The discussed case of small transverse field may be of interest for understanding the dielectric measurement and neutron scattering data for quasi-one-dimensional hydrogen-bonded ferroelectrics. However, detailed comparison with experimental results demands an introducing of weak interchain interactions (see [24,26]) that requires a separate study.

Next example regards to thermodynamics of the isotropic  $XY$  chain ( $J_j^{xx} = J_j^{yy} = J_j$ ,  $J_j^{xy} = J_j^{yx} = 0$ ) with the random intersite couplings given, for example, by the Lorentzian probability distribution density  $p(\dots, J_j, \dots) = \prod_{j=1}^N \frac{1}{\pi} \frac{\Gamma}{(J_j - J_0)^2 + \Gamma^2}$  and the transverse fields that depend linearly on surrounding couplings  $\Omega_j - \Omega_0 = \frac{a}{2}(J_{j-1} + J_j - 2J_0)$ ,  $|a| \geq 1$ . In Ref. [20] the random-averaged density of states  $\overline{\rho(E)}$  was calculated that yielded thermodynamics of the model. In particular, it was shown that the introduced randomness may cause the appearance of non-zero averaged transverse magnetization  $\overline{m_z} = -\frac{1}{2} \int_{-\infty}^{\infty} dE \overline{\rho(E)} \tanh \frac{\beta E}{2}$  at zero averaged transverse field  $\Omega_0 = 0$  ( $\overline{\rho(E)}$  is not symmetric with respect to the change  $E - \Omega_0 \rightarrow -(E - \Omega_0)$  and at  $T = 0$   $-2\overline{m_z} = \int_{-\infty}^0 dE \overline{\rho(E)} - \int_0^{\infty} dE \overline{\rho(E)} \neq 0$ ). We considered the described model for  $N = 15000$  with  $J_0 = 1$  for  $a = \pm 1.01$  with the Lorentzian and Gaussian random couplings (the probability distribution for the latter case reads  $p(\dots, J_j, \dots) = \prod_{j=1}^N \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(J_j - J_0)^2}{2\sigma^2}\right]$ ) and presented the results of computations for one random realization in Fig. 2. The displayed results are in complete agreement with the ones derived analytically for the Lorentzian disorder. However, the developed numerical procedure allows to study an arbitrary disorder. The performed calculations have indicated the appearance of  $\overline{m_z} \neq 0$  for  $\Omega_0 = 0$  at low temperature for the correlated disorder. This can be clearly demonstrated by the results of calculation of a number of negative and positive eigenvalues  $\Lambda_k$  (2)  $\mathcal{N}_-$  and  $\mathcal{N}_+$ , since at  $T = 0$   $-2\overline{m_z} = \frac{\mathcal{N}_- - \mathcal{N}_+}{N}$ .

Putting  $a = 1.01$  for a certain Gaussian random realization with  $\sigma = 0.25(1)$  that yields  $\frac{1}{N} \sum_{j=1}^N J_j = 0.999757$  (0.999027) we found  $\mathcal{N}_- = 7192(6024)$  and  $\mathcal{N}_+ = 7808(8976)$ . Another Gaussian random realization with  $\sigma = 0.25(1)$  that yields  $\frac{1}{N} \sum_{j=1}^N J_j = 1.000118$  (1.000473) gave  $\mathcal{N}_- = 7187(6073)$  and  $\mathcal{N}_+ = 7813(8927)$ . These results definitely point out the appearance of "spontaneous magnetization" due to disorder.

We end up with the calculation of the  $zz$  dynamic structure factor  $S_{zz}(\kappa, \omega) \equiv \sum_{n=1}^N e^{i\kappa n} \int_{-\infty}^{\infty} dt e^{-\varepsilon|t|} e^{i\omega t} \left( \langle s_j^z(t) s_{j+n}^z \rangle - \langle s_j^z \rangle \langle s_{j+n}^z \rangle \right)$  for the Ising chain ( $J_j^{xx} = J = 1$ ,  $J_j^{xy} = J_j^{yx} = J_j^{yy} = 0$ ) in the random transverse field defined by the probability distribution density  $p(\dots, \Omega_j, \dots) = \prod_{j=1}^N [x\delta(\Omega_j) + (1-x)\delta(\Omega_j - 0.5)]$ ,  $0 \leq x \leq 1$ . We computed the correlation functions  $4\langle s_{100}^z(t) s_{100+n}^z \rangle = \langle \varphi_{100}^+ \varphi_{100}^- \rangle \langle \varphi_{100+n}^+ \varphi_{100+n}^- \rangle - \langle \varphi_{100}^+(t) \varphi_{100+n}^+ \rangle \langle \varphi_{100}^-(t) \varphi_{100+n}^- \rangle + \langle \varphi_{100}^+(t) \varphi_{100+n}^- \rangle \langle \varphi_{100}^-(t) \varphi_{100+n}^+ \rangle$  for 250 random chains of 200 spins, performed the integration over time  $t$  with  $\varepsilon = 0.005$  and the summation over neighbours  $n$ . The obtained random-averaged  $zz$  dynamic structure factor that for  $\kappa = 0$  is presented in Fig. 3. The depicted plots demonstrate how the frequency-dependent  $zz$  structure factor rebuilds from the Ising type behaviour to the transverse Ising type behaviour as the concentration of sites with transverse field increases from 0 ( $x = 1$ ) to 1 ( $x = 0$ ). The obtained dynamic structure factor exhibits a lot of structure that is induced by the disorder arrangement of two values of transverse field 0 and 0.5. It appears that each well-defined peak for small concentrations of  $1 - x$  is connected with  $S_{zz}(0, \omega)$  for a certain chain determined by local environment of spin at  $j = 100$  (for example,  $\dots 000\dots$ ,  $\dots 0\Omega 00\dots$ ,  $\dots 0\Omega 0\dots$ ,  $\dots 0\Omega\Omega 00\dots$ ,  $\dots 0\Omega\Omega 0\dots$ ,  $\dots 0\Omega\Omega\Omega\dots$  etc., the transverse field  $\Omega_{100}$  is written in bold font, not written  $\Omega_j$ s do not influence  $S_{zz}(0, \omega)$ ). With decreasing of  $x$  a number of possible local structures in the vicinity of  $j = 100$  (and thus a number of peaks) increases and the peaks appear almost at all frequencies. However, the difference in their heights is conditioned by the probability of their appearance that is large. As a result one gets fine structure that transforms into the smooth curve only in the limiting case  $x = 0$ . The described random model has a simple interpretation in connection with partially deuterated quasi-one-dimensional hydrogen-bonded ferroelectrics. However, a study of relevant there  $xx$  spin dynamics is more cumbersome and will be reported separately.

In summary, we have presented the numerical approach suitable for calculation of time-dependent correlation functions for non-random and random spin- $\frac{1}{2}$   $XY$  chains. We have illustrated the numerical procedure deriving some new results. It is relevant to mention here the papers [36,37] devoted to numerical calculations of the  $xx$  time-dependent spin correlation functions for the isotropic  $XY$  model. The authors used explicit expressions for the elementary contractions (in contrast to our formulae that also fit the random models) and computed determinants of corresponding antisymmetric matrices that yielded only the square of correlation functions (this causes some difficulties in further calculation of the dynamic structure factor or susceptibility as well as in the study of random models). We hope that the numerical analysis of the properties of spin- $\frac{1}{2}$   $XY$  chains will be useful for understanding the results of

the corresponding measurements on quasi-one-dimensional hydrogen-bonded ferroelectrics like  $\text{CsH}_2\text{PO}_4$ ,  $\text{Cs}(\text{H}_{1-x}\text{D}_x)_2\text{PO}_4$ ,  $\text{PbHPO}_4$ ,  $\text{PbH}_{1-x}\text{D}_x\text{PO}_4$  (neutron scattering, dielectric measurement) and  $J$ -aggregates (absorption and emission spectra). However, a comparison of theoretical predictions and experimental data requires further studies.

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FIG. 1. The dynamic structure factor for the Ising chain in transverse field. (a)  $S_{xx}(\kappa, \omega)$  vs.  $\omega$  at  $\beta = 5$  for  $\kappa = 0, \frac{\pi}{4}, \frac{\pi}{2}, \frac{3\pi}{4}, \pi$  (curves 1, ..., 5, respectively) and (b)  $S_{xx}(0, \omega)$  vs.  $\omega$  for  $\beta = 5, 4, 3, 2, 1, 0.1, 0.001$  (curves 1, ..., 7, respectively).

FIG. 2. The density of states and transverse magnetization for the isotropic  $XY$  chain with random couplings and transverse fields that depend linearly on surrounding couplings.  $\rho(E)$  vs.  $E - \Omega_0$  (a,c) and  $-\overline{m_z}$  vs.  $\Omega_0$  at  $\beta = 100$  (b,d) for the Lorentzian (short dashed lines) and Gaussian (solid lines) disorder with  $\Gamma = \sigma = 0.25$  (a,b) and  $\Gamma = \sigma = 1$  (c,d); the results for non-random case  $\Gamma = \sigma = 0$  are depicted by long dashed lines.

FIG. 3. The frequency dependence of the averaged dynamic structure factor  $\overline{S_{zz}(0, \omega)}$  for the Ising chain in random transverse field at  $\beta = 5$ .







